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THE STABILITY OF CRYSTAL LATTICES

V. Zhdanov and L. Tikhonova
Siberian Physico-Tech Inst
Tomsk State U
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[Figures referred to are appended.]

The stability of a monatomic cubic face-centered crystal lattice during unilateral compression and extension is discussed. It is shown that the collapse of a lattice during compression and extension has an essentially distinct and definite character and that the lattice resists compression considerably less than it resists extension.

1. It is well known that residual inelastic strains in macroscopic solids are a secondary result of the collapse of microscopic crystal lattices in certain minute regions, which appear initially as regions of overstrain. Stepanov, for example, showed experimentally that the phenomenon of the collapse in solids consists of two phases: (1) the appearance of centers of disintegration or collapse "nuclei" and (2) the development of these minute nuclei into a macroscopic formation.

In those regions serving as collapse nuclei or centers of disintegration in solids, stress and strain evidently can attain large values. It can be assumed that the mechanical stability of these regions and the maximum inelastic deformations attain the same values as those calculated from the theory of crystal lattices. Insofar as the behavior of these regions of overstrain is determined by the development of plastic strains and fractures, it is essential to know the conditions governing stability in ideal crystal lattices for various conditions of stress. These conditions should determine the maximum stress at which the lattice can still be elastically deformed (defining the stability of the lattice), and its maximum elastic deformations.

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They should also shown how an ideal crystal lattice collapses when stress exceeds the maximum permitted for elastic stress values. Of course, a theory based on the concept of an ideal crystal lattice cannot fully explain the dynamics of collapse in a lattice, but an idea of the initial phase of disintegration in a collapsing lattice can be completely developed.

Because of the rather large elastic strains in the regions of overstrain, deformations naturally cannot be described by the theory of elasticity as based on Hooke's law. Nonlinear terms can be introduced into Hooke's law to describe such strains, as was done by Murnaghan in the case of a continuous medium and by Fuerth for cubic crystal lattices. These authors supplemented Hooke's law with second-order terms relative to components of homogenous strains. For these problems, such a generalization yields five constants characterizing the elastic properties of material, instead of the two in Hooke's law. However, elastic strains in an ideal lattice can be so large, e.g., amounting to one third of the initial volume, that calculations of only the first-order and second-order terms, and the discarding of third-order terms and above will become baseless. The calculation of still higher-order terms will lead to new constants of elasticity in such large numbers that their physical significance and the description of elastic properties of solids will be vague.

It seems more expedient to us, in cases of great stresses and strains, to use Hooke's law, i.e., "linear" relationships between stress components and strain components, taking into account the dependence of ordinary coefficients of elasticity (according to Fuerth's first-order coefficients of elasticity) upon strain or stress.

From this point of view, the coefficients of elasticity lose their significance as characteristics of the material itself and become functions of stress; but with their help we can draw an ordinary "classical" picture of the elastic properties of a solid in a strained state without requiring new coefficients of elasticity (second-order coefficients and higher).

2. A condition governing stability in crystal lattices is positive free energy, considered as a quadratic function of the components of unilateral strain of the lattice, preliminarily deformed by external stresses. These are represented by positive coefficients of elasticity in the determinant and its chief minors. Because the determinant is of the sixth degree, there will be a total of six conditions governing stablity, expressed by the coefficient of elasticity. A specific physical significance can be attached to each of the conditions governing stability; therefore during the collapse of this or that condition the lattice will collapse in a specific manner. The nature of the collapse of the lattice is evidently determined by that condition governing stablity which is the first to collapse.

3. In the present work we shall consider the stability of a monatomic cubic crystal lattice under monoaxial stress -- unilateral compression or extension along one of the edges of an elementary nucleus

We shall set the coordinate axes along the edges of an elementary lattice cube and set the stress along the Z-axis so that

$$X_x = Y_y = 0, \quad Z_z = P, \quad Y_z = Z_x = X_y = 0. \qquad (1)$$

Then the elementary nucleus takes on the form of a rectangular parallelepipedon and the lattice assumes tetragonal symmetry; the lattice will be characterized by six coefficients: C_{11}, C_{33}, C_{44}, C_{66}, C_{12}, C_{23}. With this we obtain the following conditions of stability:

$$1)\ c_{11}-c_{12}>0;\quad 2)\ c_{11}+c_{12}>0;\quad 3)\ (c_{11}+c_{12})c_{33}-2c_{23}^2>0;$$
$$4)\ c_{11}>0;\quad 5)\ c_{33}>0;\quad 6)\ c_{44}>0;\quad 7)\ c_{66}>0. \tag{2}$$

We assume that the energy of interaction of two particles is expressed in the form

$$\varphi=\frac{\varphi_0 nm}{n-m}\left\{-\frac{1}{m}\left(\frac{r_0}{r}\right)^m+\frac{1}{n}\left(\frac{r_0}{r}\right)^n\right\}, \tag{3}$$

where φ_0 is the energy of dissociation of the diatomic molecule; r_0 is the equilibrium distance in the molecule and r is the distance between interacting particles.

For numerical calculations we assume $m,n = 6,12$. In view of the problem's symmetry, the parameters of state can be selected as the length a of the edge perpendicular to stress and the ratio α of the length of the edge, parallel to stress, to the length a.

In their work Zhdanov and Konusov briefly discussed a method of calculating the elasticity of a crystal lattice as a function of the stress upon it, and set up general formulas for the equation of state and coefficients of elasticity. The general formulas were quite unwieldy; therefore we shall state here only the simpler formulas for the case of temperatures near absolute zero.

The equations of state then will be:

$$S_{m+2}^{(1)}-S_{n+2}^{(1)}\eta=0,$$
$$K\left(S_{m+2}^{(3)}-S_{n+2}^{(3)}\eta\right)=p/p_0, \tag{4}$$

and the coefficients of elasticity:

$$c_{11}/p_0=K\left\{(n+2)S_{n+4}^{(11)}\eta-(m+2)S_{m+4}^{(11)}\right\},$$
$$c_{33}/p_0=K\left\{(n+2)S_{n+4}^{(33)}\eta-(m+2)S_{m+4}^{(33)}\right\}-p,$$
$$c_{44}/p_0=K\left\{(n+2)S_{n+4}^{(23)}\eta-(m+2)S_{m+4}^{(23)}\right\},$$
$$c_{66}/p_0=K\left\{(n+2)S_{n+4}^{(12)}\eta-(m+2)S_{m+4}^{(12)}\right\}, \tag{5}$$
$$c_{12}=c_{66},\qquad c_{23}=c_{44}.$$

Here

$$\eta=(a_0/a)^m,\quad K=(1/2\alpha)[nm/(n-m)]\eta^{(m+3)/(n-m)}, \tag{6}$$

$$S_n^{(\beta\gamma\delta)}=2^{n/2}\sum_{n_1,n_2,n_3}\frac{n_1^{2\beta}n_2^{2\gamma}(\alpha n_3)^{2\delta}}{(n_1^2+n_2^2+\alpha^2 n_3^2)^{n/2}}. \tag{7}$$

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$p = p/\gamma a_0$, γ is the structural coefficient, equal for a face-centered lattice to $1/4$; $a_0 = r_0\sqrt{2}$.

A somewhat modified method of Born and Fuerth was used to calculate the sums. This method requires that the sum's first few terms, corresponding to the initial layers of particles, be summed directly and then the remaining terms be approximately summed by integration. Now we take into account the first two layers of particles in the crystal. During intégration relative to the remaining layers, the limits of integration, in contrast to [5], are determined from the values of the corresponding sums for cubic lattices. Such accuracy in calculating sums proved to be inadequate only for great compressive stresses, when the particles of the second and third layers began to play an identical role.

In 1944, we obtained the formulas for the equations of state and coefficients of elasticity in this problem; we employed them to study the temperature relation of coefficients of elasticity in lattices, taking into account the two layers of particles.

4. The equations of state (4) permit establishing a relation between the parameters of state p, α, a and T. Here we confine ourselves to the consideration of the dependence of α on stress.

The equations of state for the case of temperatures near absolute zero give a relation between stress p (in units of p_0) and α as shown in Figure 1 (the continuous curve). As is evident from the graph, the deformation within the limits $0.85 \leq \alpha \leq 1.3$ is the elastic deformation of the lattice; the maximum stresses of compression and extension can be defined as the measure of lattice stability, because beyond the maximum, deformation will take place even for smaller values of stress. We shall conditionally call these stabilities the absolute stability at compression and the absolute stability at extension; they are respectively equal to $3.3p_0$ and $10.5p_0$, as seen in Figure 1.

The curve in Figure 1 is asymmetrical; the deformation and, particularly, the resistance of the lattice during extension is considerably greater than the deformation and resistance of the lattice during compression. During extension, the size of the lattice increases considerably, up to 33 percent, and the space between particles in the direction of extension increases still more. The lattice can be assumed to collapse because of the weakening of the connective forces between particles in the direction of extension.

During compression the size of the lattice changes very insignificantly (up to 0.5 percent). It is not difficult to see that this change in distribution of particles leads to essential changes in their coordination; namely, to the transition from a face-centered lattice ($\alpha = 1$) to a volume-centered lattice ($\alpha = 1/\sqrt{2} = 0.71$). Actually, as can be seen in Figure 2, the cubic face-centered lattice ($\alpha = 1$) can be regarded as a volume-centered tetragonal lattice with a ratio of edges ($\alpha = \sqrt{2}$). A volume-centered cubic lattice is obtained during compression of a tetragonal lattice in the direction of the large edge to the values $\alpha = 1$ and $\alpha = 1/\sqrt{2}$.

Figure 1 (the continuous curve) shows that if this compression is accomplished by quasi-static means, we obtain a free lattice ($\alpha = 1/\sqrt{2}, p = 0$). But a cubic volume-centered coordination of particles, as was shown by Born and Misra, cannot exist under the selected law of interaction (3) and the condition of stability $c_{11} - c_{12} > 0$ is not fulfilled. Therefore during compression a transition from a stable coordination of

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particles to an unstable one takes place, with a surmounting of a small force (energy) barrier. The nature of the collapse in a crystal lattice during extension proves to be very dissimilar from the case for compression.

Fuerth solved the problem of unilateral extension of a cubic face-centered lattice at a temperature of absolute zero. Figure 1 shows the dotted curve obtained from formula 33 of his work. When Fuerth calculated this curve, he discarded the factor 2, so that the figures in columns 2 and 3 of Fuerth's Table 1 must be doubled. In our Figure 1 this adjustment was made. The slight separation of the curves in the right portion of Figure 1 is explained somewhat differently by our calculation of sums, which we have already mentioned. In the left portion of the graph the separation is considerable and significant, since according to Fuerth's data the face-centered cubic lattice, during compression, does not transform into a free cubic volume-centered lattice, as should happen.

According to the data of Born and Misra on the problem of central forces expressed in the form of a binomial (3), the volume-centered cubic lattice will be stable if $n<7$ and unstable if $n \geq 7$. The consideration of the first case should result in an essentially different relation of $p(\alpha)$, from that given in Figure 1. During compression of a face-centered lattice a stable volume-centered lattice should occur; that is, the tangent of the curve $p(\alpha)$ at the point $\alpha = 1/\sqrt{2}$ should be positive and hence the curve should have the form as shown in Figure 3. Deformation due to compression according to the curve in Figure 3, should lead not to simple collapse in the cubic face-centered crystal lattice, but to its polymorphous transformation into a volume-centered lattice.

Thus the problem of central forces can distinguish two types of face-centered cubic lattices; lattices of one type collapse during unilateral compression and lattices of the other type undergo polymorphous transformation.

Peng and Power studied the stability of a monatomic face-centered cubic lattice (m, n, = 6, 12) relative to extension (and compression) along the major diagonal of a cube. They established that during extension, the face-centered lattice passes into a free simple lattice and that with further extension the free simple lattice passes into a volume-centered one. Considering the lattice energy as a function of the parameter of extension λ, they further found that face-centered and volume-centered lattices are stable because they correspond to minimum energy and that a simple lattice is unstable because it corresponds to maximum energy. As a matter of fact, the energy surface at the point of the volume-centered lattice forms a saddle -- a minimum relative to the parameter of Peng and Power and a maximum relative to other parameters and in particular to our parameter α ; therefore, such a lattice for the law of forces given above is unstable.

5. We shall now investigate the conditions of stability (2).

a. 3) $c_{11}-c_{12}>0$, 5) $c_{23}>0$, 6) $c_{44}>0$. All these conditions have a tendency towards disruption during extension. This tendency is lacking or weakly expressed during compression. Figure 4 shows the left parts of conditions 3), 5), 6), for T=0. The change in pressure was taken in the range determined by the equations of state.

The expression $C_{11} - C_{12}$ equals the coefficient of shear in the plane of the "face of a rhombic dodechahedron"; $C_{11} - C_{12}$ during extension decreases to zero at $p/p_0 = 8.5$ and thereupon becomes negative. Consequently, during extension the lattice decreases its resistance to elastic shear in the plane of the face of the rhombic dodecahedron and at $p/p_0 = 8.5$ loses stability relative to these shears. The stress at which $C_{11} - C_{12}$ becomes zero, we shall conditionally call the "third" stability of the lattice.

The coefficient C_{33} characterizes the resistance of the lattice to extension parallel to the basic stress. By increasing the extension stress the coefficient decreases, but remains positive for all values of pressure, and becomes zero at $p = p_{max}$. Thus at $T = 0$ the "fifth" stability agrees with the absolute stability of the lattice. The coefficient C_{44} is characterized by resistance to shear in the plane of the face of the cube, perpendicular to the applied stress p. As can be seen in Figure 4, the lattice does not lose stability relative to such shear, although its resistance can be greatly weakened.

b. 7) $C_{66} > 0$. This condition of stability has a tendency to disruption during compression of the lattice. The left part of this condition for $T = 0°$ is represented in Figure 4.

Coefficient C_{66} characterizes resistance to shear in the plane of the face of the cube, parallel to the basic stress p. The graph clearly shows that the lattice remains stable relative to these shears, although the resistance to such shears during the presence of "basic" compression is weakened.

c. 1) $(C_{11}+C_{12})C_{33}-2C_{23}^2>0$. This condition has a strong tendency toward disruption in case of great compressive and extensional stresses.

d. 2) $C_{11}+C_{12}>0$, 4) $C_{11}>0$. The left parts of these conditions of stability, for all values of pressure, remain quite large. Therefore, their investigation is not essential.

Thus investigations of conditions of stability yield the following conclusions:

Extension -- During extension the lattice collapses because of shears in the plane of the face of a rhombic dodecahedron; the corresponding "third" stability appears as the lowest of all the stabilities of the lattice.

Compression -- In the case of compression the accuracy of calculation (accuracy of calculating sums) proved to be inadequate. Therefore no definite conclusions can be made concerning the character of lattice collapse during compression. Because the first condition is disrupted during compression in the limits of absolute stability, collapse can be assumed to take place by the appearance of a complex coordination of the particles. This can be confirmed by the ultimate compression -- the appearance of a free volume-centered lattice.

We did not investigate the important problem of the simultaneous influence of monobasic stress and temperature upon elastic characteristics and stability of the lattice. This problem will be investigated separately.

We wish to thank Professor Ya. I. Frenkel' for his valuable comments during preliminary discussion of this work.

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[Appended figures follow.]

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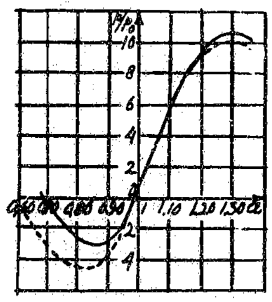

Figure 1. The relation between the parameters of equilibrium of the lattice. Volume-centered lattice is stable.

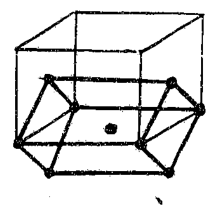

Figure 2. Formation of a volume-centered lattice from a face-centered one.

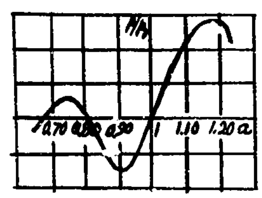

Figure 3. The relation between the parameters of equilibrium of the lattice. The volume-centered lattice is stable.

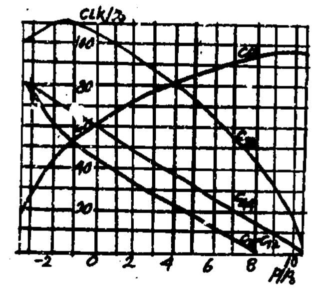

Figure 4. Coefficient of elasticity as a function of stress (p/p_0).

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